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S.B. Pope

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Direct numerical simulations of turbulence are being performed to study fundamental processes of turbulent combustion. In the flame-sheet regime of turbulent premixed combustion an important process is the stretching and bending of the surface by the turbulence. These processes have been comprehensively studied for material surfaces, and a similar study for propagating surfaces is nearing completion.

A new closure methodology recently proposed by Kraichnan holds much promise for turbulent reacting flows. An analytic solution to the model equations has been obtained; and it is found that the results are in remarkable agreement with those from our earlier direct numerical simulations.

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INTRODUCTION

There are many facets to the problem of turbulent combustion. While many aspects of the problem can now be handled satisfactorily, a remaining difficulty is the microscale processes. These can be viewed in different ways. In terms of the fundamental conservation equations, the microscale processes are mixing and reaction. The essence of the problem is that (in the appropriate regime) these processes are strongly coupled — rapid reaction being intimately connected with rapid mixing, for example. In the alternative view, combustion occurs on thin flame sheets. Then the issues are to understand the statistics and dynamics of these sheets. The sheets are convected, bent and stretched by the turbulence, and their local propagation speed is influenced by the local straining and curvature.

In this study, Direct Numerical Simulations (DNS) of turbulence are used to study basic microscale processes. Even with current supercomputers, the parameter-range accessible to DNS is quite small. If an inhomogeneous flow (e.g. a flame or mixing layer) is simulated by solving the basic conservation equations, then the practically-interesting parameter range cannot be reached. In particular a good separation between micro and macro scales cannot be achieved, while (at the same time) maintaining a large Karlovitz number. Instead we study inert homogeneous turbulence and extract information directly relevant to turbulent combustion.

In previous work (Yeung, Girimaji & Pope 1989, Pope, Yeung & Girimaji 1989) we have studied the straining and curvature of material surfaces — which, in appropriate limits, are statistically identical to flame sheets. The accomplishments in this reporting period — described below — are in four areas. The first two provide more information on material surfaces and related quantities; the third is an extension of these studies to propagating surfaces; and the fourth, separate, contribution is concerned with molecular mixing.

ACCOMPLISHMENTS

Material Element Deformation

In Girimaji & Pope (1989a) the previous studies of material surface elements is extended in two ways: first, additional important statistics are reported; and, second, material line and volume elements are also considered. The major findings are now itemized.

1. The growth rates of line and surface elements are significantly less (by a factor of about 3) than previous estimates (Monin & Yaglom 1975).
2. The smaller growth rates are due to the poor alignment between material elements and the turbulent straining motions. The lack of alignment is caused both by the action of vorticity to rotate the elements, and because the principal axes of the strain-rate rotate quite rapidly. In other words, contrary to conventional wisdom, we find that strain is fleeting rather than persistent.
3. An initially spherical infinitesimal volume element is deformed by the turbulent straining into an ellipsoid. The most probable shape of this ellipsoid is like a squashed cigar — one axis is extended, another equally compressed, while the third remains (approximately) unchanged.

Stochastic Model for Velocity Gradients

Any quantity related to material element deformation — the straining on a material surface, for example — can be calculated from the velocity-gradient time series following a fluid particle. Thus the study of material element deformation described in the previous subsection was performed using the velocity-gradient time series obtained from DNS.

We have devised a computationally-simple stochastic model for the velocity-gradient time series that reproduces the major statistics of the DNS time series. This stochastic model can be used in turbulent combustion models (e.g. that of Pope & Chen 1988) to calculate the strain rate on the flame sheet etc.

The stochastic model (fully described and tested by Girimaji & Pope 1989b) is a tensor-valued diffusion process. Thus it is a Markov process with continuous sample paths. The drift and diffusion coefficients in the model have been determined — partly analytically, partly empirically — by requiring that the most important statistics of the process match those obtained from DNS. Typically the model is accurate to within 15%.

Propagating surfaces

The material surfaces described so far represent flame sheets only in special limits. In the context of premixed flames, the limit is $u_L/u_\eta \to 0$, where u_L is the laminar flame speed and u_η is the Kolmogorov velocity scale.

We have nearly completed a study of propagating surfaces, with propagation speeds u_L of $u_L/u_\eta = 0, \frac{1}{4}, 1, 4, 16$. The study of propagating surfaces ($u_L>0$) is much more difficult than that of material surfaces ($u_L=0$), because of cusp formation. That is, the curvature of a surface element can become infinite in finite time.

The first difficulty to be faced is to devise an accurate and stable numerical algorithm that can calculate the surface properties up to the point of cusp formation. This requires special consideration of the singularity (i.e. the cusps). Such an algorithm has been devised. It is second-order accurate, and reduces to an exact analytic solution as the singularity is approached.

Because of the formation of cusps, the time series of surface properties are finite in duration, and they are inherently non-stationary. Thus the second difficulty is the analysis of these time series — as compared to the stationary time series of arbitrarily long duration for material surfaces.

The preliminary results confirm expectations. For example, the Lagrangian time scales and the straining on the surface decrease with increasing u_L/u_η. The precise variation of these statistics — yet to be quantified — is of fundamental importance to theoretical questions of premixed flame propagation. Also as expected, the mean time to cusp formation decreases with increasing u_L/u_η.

The major effort for the first 6 months of 1990 will be to finalize and report the results of this study of propagating surfaces.

Kraichnan's PDF Model

For decades to come, direct numerical simulation will not be used as an engineering design tool for turbulent combustion devices, because the computation demands are way beyond reach. Instead, our philosophy is to use DNS to guide and test the development of statistical models that can be used as design tools. For turbulent combustion the most favorable statistical approach is the pdf method (see, e.g. Pope 1985).

In the pdf approach, while complex reactions can be treated without approximation, mixing — i.e. molecular diffusion processes — have to be modelled. For the last 15 years the development of a completely satisfactory mixing model has proved an allusive objective. Recently Kraichnan (1989) has proposed a completely new modelling methodology which appears to be a breakthrough. As described in the following paragraphs, we have obtained an analytic solution to Kraichnan's model equations which are in spectacular agreement with our previous DNS results. First these DNS results are reviewed.

Eswaran & Pope (1988) (work supported by AFOSR 85-0083) performed direct numerical simulations of the decay of an inert passive scalar $\phi(\underline{x},t)$ in stationary, homogeneous, isotropic turbulence. The initial condition corresponds to blobs of scalar with $\phi \approx 1$ and an equal quantity of blobs with $\phi \approx -1$. Thus the initial pdf of ϕ, $f(\psi)$, corresponds, approximately, to the double-delta-function distribution.

$$f(\psi) = \frac{1}{2}\left[\delta(\psi+1) + \delta(\psi-1)\right] . \qquad (1)$$

The results show that the decay of the scalar variance depends on the size of the initial blobs (relative to the turbulence scales) — consistent with experimental observations. However, it is found that the shapes adopted by the pdf's are independent of blob size. Figure 1 shows the pdf's obtained from the DNS for three different values of the initial blob size. It may be seen that the shapes are essentially the same in each of the three figures (Figs. 1a,b,c).

Kraichnan's model is conceptually simple, though technically difficult. The idea is to map the non-Gaussian scalar field $\phi(\underline{x},t)$ to a Gaussian field $\phi_o(\underline{x},t)$ by a mapping $Y(\bullet,t)$: i.e. $\phi_o(\underline{x},t) = Y(\phi[\underline{x},t],t)$. Gaussian closure approximation are then applied to the Gaussian field ϕ_o.

For the case of an inert passive scalar with the initial condition given by Eq. (1) we have obtained the following analytic solution to Kraichnan's model:

$$f(\psi;t) = \frac{1}{2} \Sigma \exp\{-\frac{1}{2}\, \psi_o^2\, (1-\Sigma^{-2})\} \,. \qquad (2)$$

where

$$\Sigma^2 = e^{t^*}-1 \,,$$

$$\psi_o = \sqrt{2}\;\; \Sigma\, \mathrm{erf}^{-1}(\psi) \,,$$

and t* is normalized time. Figure 2b shows the pdf's according to Eq. (2) compared (Fig. 2a) to those from DNS. It may be seen that the agreement is remarkable. In spite of the considerable efforts of several workers over the past 15 years, no other models have come close to Kraichnan's in qualitative or quantitative performance.

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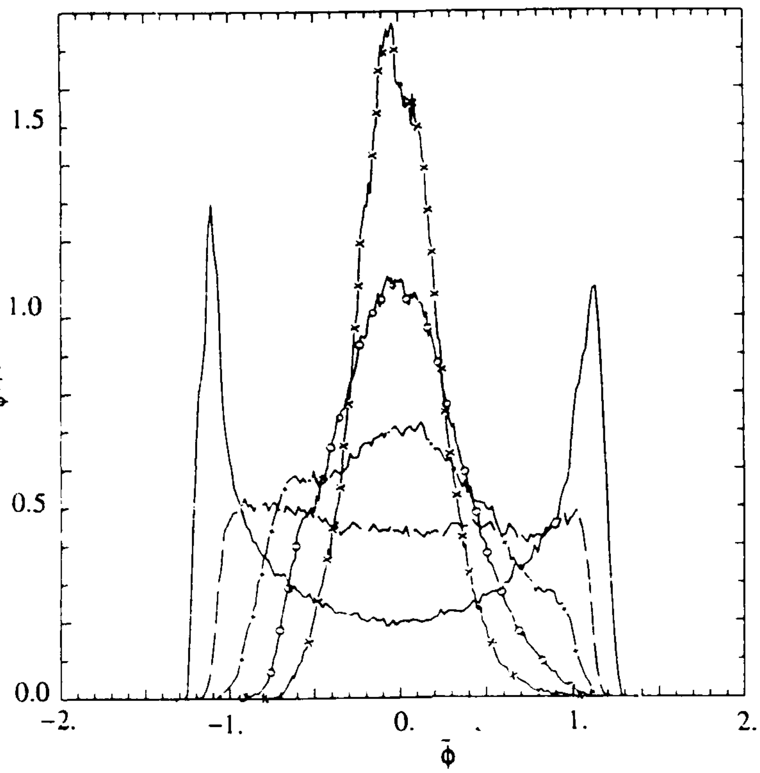
IG. 1a :The scalar pdf from simulation F2a ($Re_\lambda \approx 50$, $k_s/k_0 = 1$) at dif-
erent times. Lines: — ($tu/l = 0.22$; $\phi'/\phi'_0 = 0.99$), - - - (1.49; 0.73), - + -
2.11; 0.55), -o- (2.78; 0.40), -x- (3.47; 0.27).



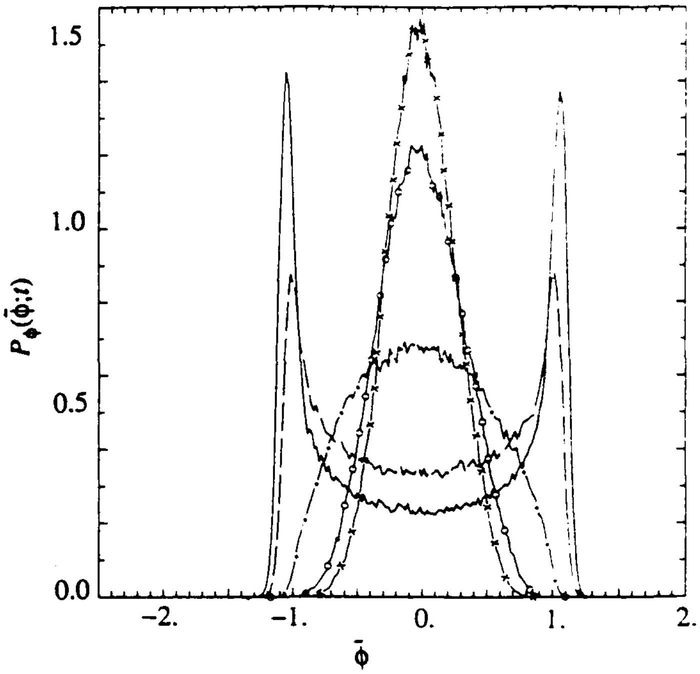


FIG. 1b :The scalar pdf from simulation F2c ($Re_\lambda \approx 50$, $k_s/k_0 = 4$) at dif
ferent times. Lines: — ($tu/l = 0.22$; $\phi'/\phi'_0 = 0.92$), - - - (0.42; 0.80), - +
(0.83; 0.54), -o- (1.28; 0.35), -x- (1.49; 0.28).

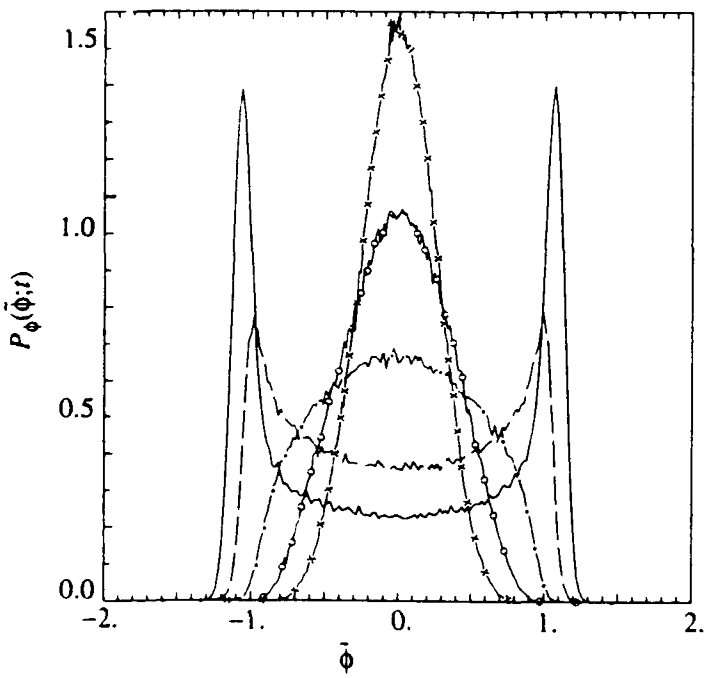
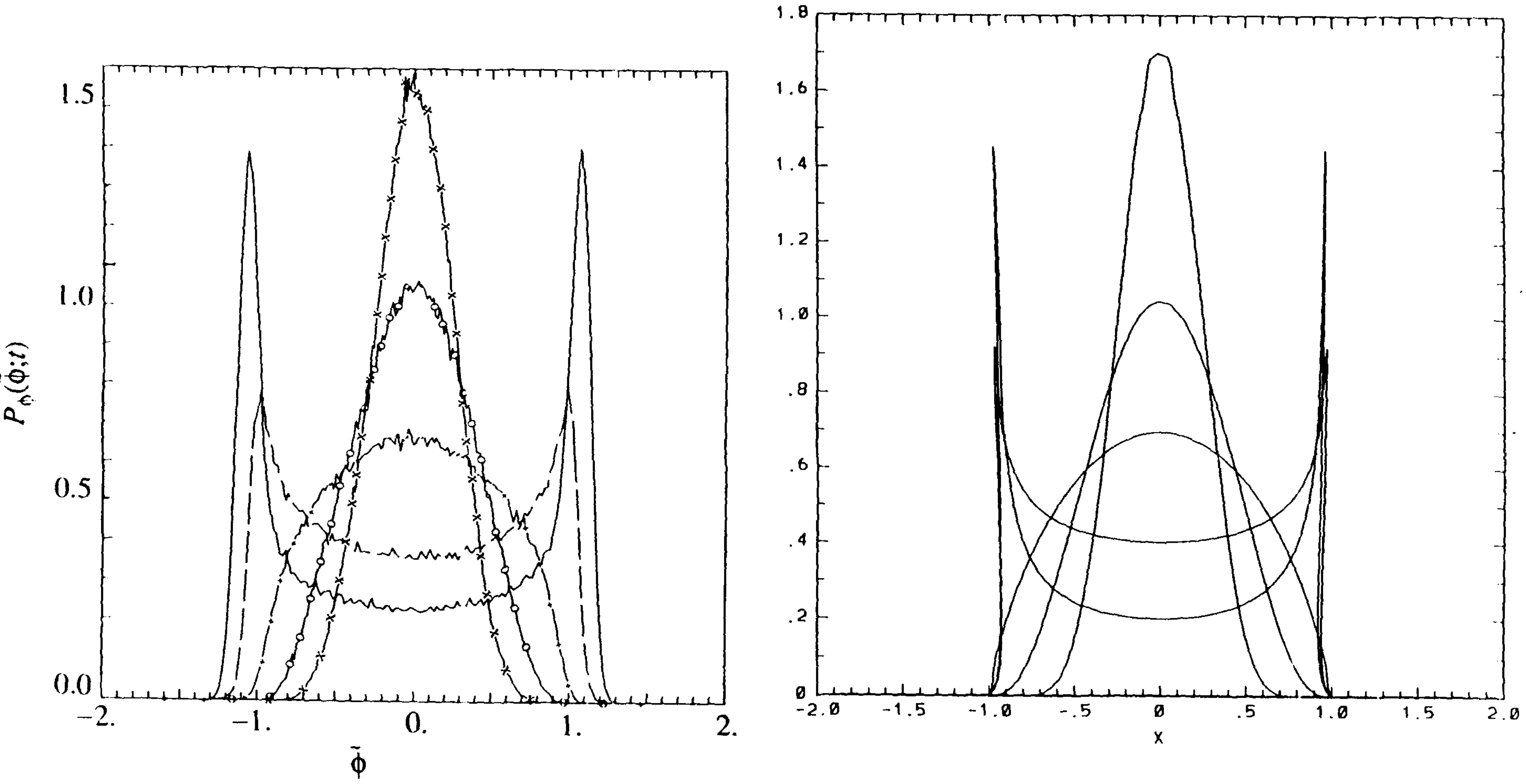


Fig. 1: Scalar pdf's from direct numerical simulations of Eswaran & Pope (1988).

FIG.1c : The scalar pdf from simulation F2e ($Re_\lambda \approx 50$, $k_s/k_0 = 8$) at dif-
ferent times. Lines: — ($tu/l = 0.07$; $\phi'/\phi'_0 = 0.94$), - - - (0.22; 0.76), - + -
(0.42; 0.54), -o- (0.62; 0.38), -x- (0.83; 0.27).



a) b)

Fig. 2: Scalar pdf's from a) DNS, Eswaran & Pope (1988), b) Kraichnan's model, Eq. (2).

PUBLICATIONS

P.K. Yeung and S.B. Pope (1989) "Lagrangian statistics from direct numerical simulations of isotropic turbulence," J. Fluid Mech., 207, 531-586. [Work performed under AFOSR85-0083; published in this reporting period.]

P.K. Yeung, S.S. Girimaji and S.B. Pope (1989) "Straining and scalar dissipation on material surfaces in turbulence: implications for flamelets," Combustion and Flame (to be published).

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PERSONNEL

Prof. S.B. Pope, Principal Investigator	0% (Spring, Sabbatic Leave) 15% (Fall)
Dr. P.K. Yeung, Ph.D. Student	1 month
Mr. S.S. Girimaji, Ph.D. Student	100%
Mr. Y.Y. Lee, Ph.D. Student	40%

DEGREES AWARDED

P.K. Yeung received his Ph.D. in 1989. He is continuing research work using DNS at Pennsylvania State University.

INTERACTIONS

The talks given and meetings attended by the P.I. during the reporting period are:

Cambridge University, Engineering Department, January 26.

Cambridge University, Applied Math, February 17.

Cranfield (Combustion Institute Meeting), April 5.

Rolls Royce, Derby, April 20.

Cambridge University (short course in PDF methods), May 5.

Imperial College, London, May 17.

University of Michigan, AFOSR meeting, June 19-21.

General Motors Research Labs, June 22.

Turbulent Shear Flows Symposium, Stanford, August 21-23.

NASA Lewis, September 14.

Vanderbilt (Sandia STAR meeting), November 6.

Arnold Engineering Development Center (Sandia STAR meeting), November 7.

APS/DFD meeting, NASA Ames, November 19-21.

INVENTIONS

None

PATENTS

None